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13. ABSTRACT

During a period of three years, several important developments and calculations were made on the electron--molecule scattering. We presented rotationally elastic, inelastic and summed cross sections for electron scattering with several polyatomic molecules (CH_4, SiH_4, GeH_4, H_2O, H_2S and NH_3) in a highly sophisticated close--coupling non--empirical theory. Exchange effects were included exactly, while polarization corrections were considered approximately but without involving any fitting parameter. Results were compared with measurements where such data were available. No previous theoretical investigation is available on these molecules in such detail and energy range.

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CONCLUSIONS

During a period of three years, several important developments and calculations were made on the electron--molecule scattering. We presented rotationally elastic, inelastic and summed cross sections for electron scattering with several polyatomic molecules (CH_4, SiH_4, GeH_4, H_2O, H_2S and NH_3) in a highly sophisticated close--coupling non--empirical theory. Exchange effects were included exactly, while polarization corrections were considered approximately but without involving any fitting parameter. Results were compared with measurements where such data were available. No previous theoretical investigation is available on these molecules in such detail and energy range.

This study has drawn several important conclusions: (1) exchange effects at the exact level and model polarization potentials can describe low energy e--molecule scattering quite accurately, (2) polarization effects should be included in a theory where target orbitals are relaxed in the presence of incoming particle, (3) the effect of gas temperature on the cross sections is crucial for rotationally inelastic channels, (4) a single--center approach can be useful for many polyatomics without any convergence problem, (5) the iterative scheme is quite promising tool in future if employed in an optimized way as suggested in this study. For the first time, a large variety of molecules are studied at intermediate and high energies. The total cross section (sum of elastic plus all possible inelastic channels) for several gases were calculated and presented in tabular form in the energy range of 10--5000 eV. Such theoretical data are not found in the literature for most of the targets studied here. In addition we also reported Born--Bethe parameters for all these molecules. An attempt was made to find a correlation between molecular properties and the corresponding total cross section quantity. Several computers codes were modified and developed in order to deal with big molecules and also polar ones. Our Single--center--expansion scheme was made possible to work for much heavier systems (e.g. GeH_4, SF_6, CF_4, etc.) than the typical CH_4, etc. ones. An interface program was developed which generates SCE quantities from

molecular wave functions. This progress was realized in terms of some actual calculations on some molecules of larger size.

This work is still in progress in two ways: (1), to investigate electron interactions in large systems, and (2) to employ the present set of programs for vibrational and electronic excitation of polyatomic molecules. Some preliminary progress has been made for the CH_4 and H_2O molecules. However, this work requires a huge amount of effort in terms of manual and computational facilities.